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Research Paper

Algorithmic robustness for contact analysis of polyhedral blocks in discontinuous deformation analysis framework

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ABSTRACT

Algorithmic robustness is important in the contact interaction analysis of polyhedral blocks using discontinuous computation methods. Several robustness issues of contact analysis associated with the identification of four contact types are discussed here, including rounding errors of floating-point operations, criteria and tolerances in contact type identification, and restrictions of input parameters. This paper also proposes revised criteria to identify contact types and general rules to specify tolerances regarding contact searches, quasi-parallel edges, overlapping angle and maximum displacement in a time step. These rules facilitate robust contact analysis of polyhedral blocks in the discontinuous deformation analysis framework.

1. Introduction

Rock with natural discontinuities behaves in a more complex manner than materials represented as a continuum. Therefore, numerical methods such as the discrete element method (DEM) [1] and discontinuous deformation analysis (DDA) [2] were proposed to investigate the static and kinetic behaviour of this material. For example, two-dimensional (2D) DDA models have been extended in theory [3–5] and successfully applied in landslide simulations [6–8], slope stability analysis [9,10], cavern excavation investigation [11], rock blasting modelling [12], wave propagation investigation [13] and hydro-mechanical modelling [14–16]. Three-dimensional (3D) DDA and DEM have been extended [17] and applied in landslide simulation [18–20], tunnel stability analysis [21–23], and particle-based rock failure simulation [24]. However, the application of 3D DDA for large-scale and complex polyhedral block systems is limited by several obstacles, including the high computational cost and the algorithmic robustness for analysis of block contact.

The computational efficiency of these methods is closely related to the contact detection algorithm and equation solver, as they consume most of the computational time in DDA. Efforts to enhance the computational efficiency for analysis of block systems include parallel and scalable block system generation [25] and OpenMP and GPU-based parallel computing implementations [26–28]. Traditional schemes for contact detection usually include two phases: a "rough" detection phase to identify all neighbouring blocks and a "delicate" detection phase to obtain the actual contact points, contact plane and contact mode for each neighbouring block pair [29–31]. The computational efficiency of contact detection is affected by the algorithms used in both phases. Some algorithms [32–34] have been proposed to efficiently establish neighbouring block pairs in the rough detection phase. Meanwhile, various algorithms have been proposed to determine the specific contact types for polyhedral blocks in the delicate search phase [35–46]. Among these, the fast direct search algorithm [36], fast common plane algorithm [38] and shortest link method [39] exhibit better efficiency for convex polyhedra than traditional direct search algorithms. When concave polyhedra are included, the direct search algorithm, which is based on four basic contact types, i.e., vertex-to-vertex (v-v), vertex-to-edge (v-e), vertex-to-face (v-f), and edge-to-edge (e-e), is commonly used, and the number of potential checked pairs can be reduced by preprocessing techniques [31,35]. Alternatively, a concave polyhedron can be decomposed into several convex polyhedra and analysed by algorithms for convex polyhedra [37].

The algorithmic robustness of contact analysis of a polyhedral block system is another crucial aspect of modelling realistic and complex jointed rock masses. Here, robust contact analysis indicates that the results of the contact algorithm are reliable and physically permissible with different block shapes and sizes and various initial conditions and computation parameters. This should be considered during both the model generation and subsequent analysis process. In block

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representation and related geometrical computation, coordinates and vectors are usually represented by floating-point numbers in a program, where the rounding error should be addressed. "Rounding error" is the difference between the exact mathematical value and its approximation due to rounding. In the block generation process, exact arithmetic may be applied to avoid the rounding error issue associated with floating-point numbers [47]. However, this is very difficult in the contact analysis, where floating-point numbers are normally adopted. Therefore, the robustness issues in contact analysis include addressing the rounding error, correctly identifying contact types, setting appropriate tolerance values for contact searches, checking non-overlap conditions, distinguishing parallel/crossing e-e contact types, and evaluating maximum block displacement and rotation.

In this paper, investigations of such robustness issues are based on a commonly used contact detection procedure [29–31,35] that considers basic types of contact, including v-v, v-e, v-f and crossing e-e. Other contact types, such as face-to-face (f-f), edge-to-face (e-f), and parallel e-e, can be regarded as combinations of these four basic types. The 2D corner-corner contact issue has been investigated [48–52], while in 3D v-v/v-e contact is usually resolved by the first entrance and shortest exit rules [29,31,53]. This paper considers several aspects of algorithmic robustness during contact analysis: (1) strictly speaking, blocks/particles contact only along their boundaries. For computational feasibility of the penalty function method [2], a small overlap/penetration should be allowed in the contact area; (2) to identify all possible contact pairs within a specified distance tolerance, the block displacements in each step should be restricted; (3) for the step-based DDA procedure, contact situations in which the contact geometrical data changes rapidly should be well investigated, as some procedures to identify contact types may introduce block penetrations. These possible penetrations should be restricted to avoid unrealistic interactions that tend to destabilize the computation; (4) in the identification of the four basic contact types, a sequence of v-v, v-e, v-f/e-e is usually followed to avoid excessive contact pairs. Each type is confirmed if it passes the distance check and no-overlap check, in which tolerances related to contact territories, overlapping angles and parallel edges are necessary; (5) in the formulation of v-f/e-e contact [53–58], omitting the high order terms when computing the normal penetration distance may lead to small perturbations (deviations from the actual solution) that should be carefully managed when determining the open/closed mode of contact pairs in an open-close iteration (OCI); (6) the rounding error associated with floating-point [59] representation of coordinates and vectors should be carefully controlled during contact analysis.

To address these issues, this paper first discusses several aspects of algorithmic robustness considerations that may have significant effects on the simulation result. Subsequently, the initial interpenetration effects are investigated to provide guidance for assignment of algorithmic tolerance. Criteria in contact identification are revised to improve the algorithmic robustness in treat contact cases involving sharp angles and quasi-parallel edges. General rules are recommended for the specifications of tolerances regarding contact searches, quasi-parallel edges, overlapping angle and maximum displacement and rotation in a time step. Examples of contact scenario of sliding block, approaching vertices and quasi-parallel edges and failure of block systems illustrate the proposed rules for the tolerance values and the revised contact territory scheme.

2. Robustness issues

The major assumptions in most 2D and 3D DDA programs [2,53–58] are summarized as follows: (1) a complete first-order approximation of block displacement; (2) an elastic deformation pattern; and (3) no tension in the contact normal direction, and the Mohr-Coulomb criterion applies to the shear behaviour of each closed contact pair. The first assumption also implies that the displacement and deformation of each block are so small that the higher order terms regarding the block rotation and block deformation can be neglected. Contact interaction can be solved in the DDA framework by various techniques, such as the penalty function method [2,53–58], Lagrange multiplier method [60], augmented Lagrange multiplier method [61] or complementary theory [62]. In contrast to the traditional penalty function scheme, the complementary form DDA [63], dual form DDA [64], and explicit contact constraints scheme [65] can solve contact interaction without using the implicit OCI process or penalty springs. In this study, however, the penalty function method with OCI process is adopted considering its efficiency.

To maintain the algorithmic robustness for contact analysis of polyhedral blocks using the penalty function method, two requirements should be satisfied in the contact detection and contact computation processes: (1) all potential contact pairs and their entrance positions should be identified in the detection process, and the relevant contact constraints should be applied to avoid large interpenetration at the end of the time step; (2) convergence of the OCI (i.e., limited tension and limited penetration) should be obtained in each step when the penalty function method is applied to manage contact constraints. The strict convergence of the OCI might not be needed [66,67], but the penetration should still be limited in those cases. Considering the above assumptions and requirements in the DDA framework, the associated robustness issues are discussed in the following sections.

2.1. Rounding errors of floating-point numbers

Coordinates of block vertices and vectors of face normals are usually represented by single-precision or double-precision floating-point numbers in computation. The judgement of floating-point values is necessary in contact detection and the OCI process. For example, the open/closed modes of contact pairs are determined by evaluating the sign of a determinant representing block penetrations, and no-overlap examinations for v-f/e-e pairs are performed by evaluating the sign of the dot product of vectors that specify the plane or edge orientations.

Usually, the single-precision computer arithmetic provides a sufficient number of digits to prevent rounding errors from affecting the contact analysis. When comparisons of floating-point numbers are necessary, setting algorithmic tolerances can avoid the rounding error effects. Instead of comparing the exact values of two floating-point numbers, comparison of their significant digits is adequate. In this study, Eq. (1) is used to determine the equality of two floating-point numbers a and b:

$$|a-b| < \varepsilon \tag{1}$$

where ε can be a small value proportional to the absolute value of a or b; the ε term can also be a strict precision, depending on the number of significant digits needed.

For comparison of "greater than or equal to" or "less than or equal to" between a floating-point number and a predefined value, the "equal to" comparison with tolerance ε can be performed first, followed by the "greater than" or "less than" comparison. For example, the open/closed mode judgement includes comparison of d_n (normal separation distance between a contact pair) with 0 (e.g., $d_n \geq 0$), and a tolerance ε proportional to d_n can be used: the contact mode is set as unchanged if $|d_n| < \varepsilon$; open if $d_n > 0$; or closed if $d_n < 0$.

2.2. Issues in contact detection

Two criteria are typically used to establish contact pairs for polyhedral blocks in contact detection processes [29,31], including the distance criterion that distinguishes contact types by measuring the distance of two blocks, and the no-overlap criterion that locates the first entrance position or shortest exit position. Several issues regarding the two criteria and tolerance values in the checking process will be investigated.